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Computational Study of Synthetic Routes Towards $PH_2BH_2EH_2$ (E = C, Si, Ge, Sn) Complexes

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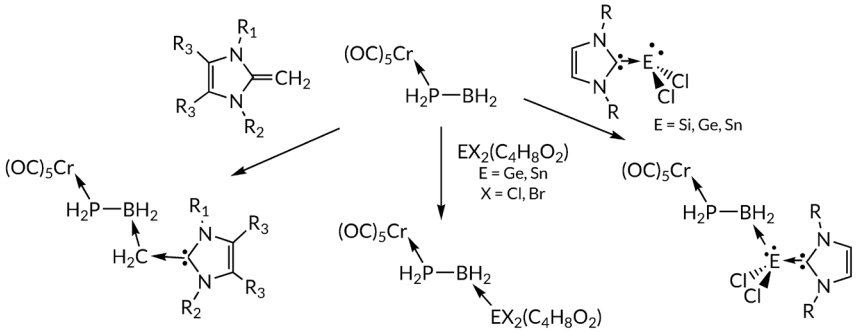
The compounds with combination of group 13/14/15 elements in a chain and only hydrogen substituents (parent compounds) are of high interest due to their potential use as single-source precursors for ternary materials for small band gap optical devices [1] and in construction of inorganic polymers – alternatives to the established organic-based polymers [2]. In contrast to parent compounds of group 13/15 and 14/15 elements, which complexes with Lewis acids and Lewis bases were synthesized, complexes of $E^{(15)}H_2E^{(13)}H_2E^{(14)}H_2$ are unknown up to now.

In order to define the optimal reagents for syntheses of $PH_2BH_2EH_2$ (E – group 14 element) complexes the computational study of three synthetic routes was carried out at B3LYP-D3/def2-TZVP level of theory (Scheme 1).



Scheme 1.

Almost all considered reactions (besides the reaction with $SnCl_2{\cdot}C_4H_8O_2$) are thermodynamically more favorable than the side processes of $Cr(CO)_5{\cdot}PH_2BH_2$ di- and trimerization with H_2 elimination in the gas phase. We propose three N-heterocyclic olefins (^{Me}IDippCH$_2$, Im(Me)(*i*-Pr)CH$_2$, Im(*i*-Pr)$_2$CH$_2$) for the synthesis of $PH_2BH_2CH_2$ complex, and $SiCl_2{\cdot}$IDipp and $GeCl_2{\cdot}$IDipp for the first step in the syntheses of $PH_2BH_2SiH_2$ and $PH_2BH_2GeH_2$ complexes.

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